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Spherical Combustion Layer in a TNT Explosion

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A theoretical model of combustion in spherical TNT explosions at large Reynolds, Peclet and Damk hler numbers is described. A key feature of the model is that combustion is treated as material transformations in the Le Chatelier plane, rather than "heat release". In the limit considered here, combustion is concentrated on thin exothermic sheets (boundaries between fuel and oxidizer). The products expand along the sheet, thereby inducing vorticity on either side of the sheet that continues to feed the process. The results illustrate the linking between turbulence (vorticity) and exothermicity (dilatation) in the limit of fast chemistry thereby demonstrating the controlling role that fluid dynamics plays in such problems.

Introduction

Considered here are turbulent combustion fields generated by the explosion of a 1-gram spherical charge of TNT. As pointed out by Anisimov and Zel'dovich [1,2], the shock-accelerated interface between the expanding detonation products and the surrounding air is unstable [3,4], and rapidly evolves into a turbulent mixing layer. Anisimov et al. identified two mixing regimes: (i) an early-time regime where the mixing layer thickness is small compared to the mean fireball radius, and (ii) a late-time regime where turbulent mixing fills the entire fireball. The evolution of the turbulent mixing layer in a non-reactive (Nitrogen) atmosphere was reported previously [5]. Described here is the reactive case—in an air atmosphere.

Formulation

The expanded detonation products from the TNT charge are rich in $C_{(s)}$ and CO which serve as a fuel; when mixed with air, they combust (after-burn) releasing another 2,500 Cal/g [6] over and above the detonation energy of 1,093 Cal/g. Combustion takes place in the turbulent velocity field of the hot combustion products, so that the oxidation rate is, in effect, controlled by the turbulent mixing rate. The model recognizes three fluids: *fuel-F* (expanded TNT detonation products), *oxidizer-A* (air), and combustion *products-P*. We consider the exothermic-flow limit [7] where Reynolds number $Re \rightarrow \infty$, Peclet number $Pe \rightarrow \infty$, Damk hler number $Da \rightarrow \infty$, and Mach number $Ma > 0$. In this limit, effects of molecular transport are small [8], and are therefore modeled as sub-grid processes. As is typical of combustion in unmixed systems, the fuel reacts with the oxidizer in stoichiometric proportions.

Multi-fluid Model

In the limit of $Re \rightarrow \infty$, the mixture, m , obeys the gas dynamic conservation laws :

$$\text{Mass:} \quad \partial_t \rho_m + \nabla \cdot (\rho_m \mathbf{u}) = 0 \quad (1)$$

$$\text{Momentum:} \quad \partial_t \rho_m \mathbf{u} + \nabla \cdot (\rho_m \mathbf{u} \mathbf{u}) = -\nabla p_m \quad (2)$$

$$\text{Energy:} \quad \partial_t \rho_m (u_m + \mathbf{u} \cdot \mathbf{u} / 2) + \nabla \cdot \rho_m (u_m + \mathbf{u} \cdot \mathbf{u} / 2) \mathbf{u} = -\nabla \cdot (p_m \mathbf{u}) \quad (3)$$

where ρ, u, p and \mathbf{u} denote the density, specific internal energy, pressure and velocity.

These are supplemented by auxiliary balance laws for mass and energy to follow the evolution of the thermodynamic variables of each fluid throughout the domain. In the limit of $Pe \rightarrow \infty$, the **mass balance equations** for the fluids acquire the form:

$$\text{Fuel:} \quad \partial_t \rho_F + \nabla \cdot (\rho_F \mathbf{u}) = -\dot{\rho}_s \quad (4)$$

$$\text{Air:} \quad \partial_t \rho_A + \nabla \cdot (\rho_A \mathbf{u}) = -\sigma \dot{\rho}_s \quad (5)$$

$$\text{Products:} \quad \partial_t \rho_P + \nabla \cdot (\rho_P \mathbf{u}) = (1 + \sigma) \dot{\rho}_s \quad (6)$$

where σ denotes the stoichiometric coefficient ($\sigma = 3.2$ for TNT-air). These equations contain source/sink terms that sum to zero thereby satisfying mass conservation (1) for the mixture.

Also in the limit of $Pe \rightarrow \infty$, the **energy balance equations** for the fluids become:

$$\text{Fuel:} \quad \partial_t \rho_F u_F + \nabla \cdot (\rho_F u_F \mathbf{u}) = -p_F \nabla \cdot \mathbf{u} - u_F \dot{\rho}_s \quad (7)$$

$$\text{Air:} \quad \partial_t \rho_A u_A + \nabla \cdot (\rho_A u_A \mathbf{u}) = -p_A \nabla \cdot \mathbf{u} - u_A \sigma \dot{\rho}_s \quad (8)$$

$$\text{Products:} \quad \partial_t \rho_P u_P + \nabla \cdot (\rho_P u_P \mathbf{u}) = -p_P \nabla \cdot \mathbf{u} + u_P (1 + \sigma) \dot{\rho}_s \quad (9)$$

These equations contain source/sink terms that sum to zero, consistent with energy conservation for the mixture (3). Combustion influences these fields through the source $\dot{\rho}_s$.

In the limit of $Da \rightarrow \infty$, the combustion zone collapses to an infinitely-thin **exothermic surface**: $\mathbf{x}_s(t)$ which acts simultaneously as a **sink** for F & A and a **source** for P . It may be represented by a Dirac delta function, δ :

$$\dot{\rho}_s(\mathbf{x}, t) \rightarrow \begin{cases} \rho_F(\mathbf{x}, t) \delta(t - t_s) & (1 \leq \lambda < \infty) \\ \rho_A(\mathbf{x}, t) \delta(t - t_s) / \sigma & (0 < \lambda < 1) \end{cases} \quad (10)$$

where t_s denotes the time when the fluid particle passes through the exothermic surface, while $\lambda(\mathbf{x}, t) \equiv [\text{Air} - \text{Fuel ratio}] / \sigma$. The meaning of this notation is:

$$\int_0^{\delta t} \int_{\delta V} \dot{\rho}_s dV dt \equiv \begin{cases} m_F / \delta V & (1 \leq \lambda < \infty) \\ m_A / (\sigma \delta V) & (0 < \lambda < 1) \end{cases} \quad (11)$$

Thermodynamic Model

Following [9], the thermodynamic properties of the fluids are represented as loci of states in the Le Chatelier diagram of specific internal energy: u_K as a function of the thermodynamic parameter: $w_K \equiv p_K v_K$ ($K = F, A, R, \& P$), as depicted in Fig. 1. The air curve, A , is based on thermodynamic equilibrium calculations [10]. The fuel curve, F , is based on CHEETAH calculations for TNT [11]. A and F mix to form reactants R according to the stoichiometric rule:

$$u_R = (u_F + \sigma u_A) / (1 + \sigma) \quad \& \quad w_R = (w_F + \sigma w_A) / (1 + \sigma) \quad (12)$$

Starting with points on R , the STANJAN code [12] was used to calculate corresponding thermodynamic equilibrium points on the products curve P . In particular, point i on R transforms to point hp on P for combustion at constant enthalpy & pressure, or to point uv on P for combustion at constant energy & volume. These curves were fit with linear functions:

$$u_A = -0.31909 + 2.65352w_A \quad \& \quad u_F = -5.28788 + 4.1405w_F \quad (13)$$

$$u_R = -1.51278 + 2.98856w_R \quad \& \quad u_P = -4.82385 + 5.40184w_P \quad (14)$$

where $[u]$, $[w] = \text{kJ/g}$. The above suggest the following form for the equations of state (EOS):

$$u_K = F_K(w_K) \cong -|q_K| + C_K w_K \quad (15)$$

Function F_K represents the general curve of Fig. 1; it is well approximated by the linear relation (15) in the domain of interest; its inverse: $F_K^{-1}(u_K)$ allows one to evaluate w_K from its specific internal energy u_K . Thus, the pressure in a pure fluid K becomes:

$$p_K = \rho_K w_K = \rho_K [u_K + |q_K|] / C_K \quad (16)$$

while for a multi-fluid cell, the mixture pressure is

$$p_m = \rho_m w_m = \rho_m [u_m + |q_m|] / C_m \quad (17)$$

which is based on the mixture properties established by the ideal mixing rules:

$$\rho_m = \sum_k \rho_K \quad \rho_m w_m = \sum_K \rho_K w_K \quad \rho_m u_m = \sum_K \rho_K u_K \quad \rho_m C_m = \sum_K \rho_K C_K w_K / w_m \quad \rho_m q_m = \sum_K \rho_K q_K \quad (18)$$

Combustion Model

The combustion model takes into account three sub-grid processes: (i) *reactants formation*: fuel and air molecularly mix in stoichiometric proportions (12) to form reactants (thus modeling sub-grid mass diffusion); (ii) *transformation in the Le Chatelier plane*: reactants are transformed into products at constant uv (for closed systems) or at constant hp (for deflagrations); (iii) *thermal equilibration*: between post-combustion fluids in the cell (thereby mimicking heat diffusion).

Application

The model was used to simulate the explosion of a 1-gram spherical TNT charge in an air atmosphere. The gas dynamic conservation equations for the mixture (1)-(3) were integrated by means of a higher-order Godunov scheme [13], while the auxiliary mass and energy balance equations for the fluids (4)-(9) were advanced as convection equations using the same Godunov scheme. Adaptive Mesh Refinement [14,15] was used to follow the mixing on the grid.

A cross-sectional view of the flow field is presented in Fig. 2. Material fields are visualized as *yellow* fuel, *blue* air and *red* combustion products. Velocity fields are visualized by means of vorticity contours (*turquoise*=positive & *chateuse*=negative) and dilatation contours (*black*=negative). Exothermic cells are marked by *white* stars. Expansion of the TNT products drives a spherical blast wave into the surrounding atmosphere [16]. The shock-accelerated interface between F & A is unstable and rapidly evolves into a turbulent mixing layer. A secondary (backward facing) shock develops due to the over-expansion of the detonation products [5]. This shock implodes at $t = 0.115\text{ms}$ thereby pulling air towards the center, forming deep Taylor cavities. Kelvin-Helmholz rollups are visible on the cavity walls. After reflection at the center, the secondary shock propagates back through the mixing layer, creating

additional vorticity due to baroclinic effects (Fig. 3). This leads to the development of distributed combustion regime where exothermic effects occur throughout the mixing layer.

Blowups of the exothermic fields near a large-scale structure are shown in Fig. 4. In this simulation, combustion is confined to thin *exothermic sheets* (boundaries between fuel and oxidizer). The exothermic sheet acts as a dilatation source—causing the products to expand *along* the sheet rather than normal to it, as in laminar flames. This generates vorticity on either side of the sheet—forming, in effect, an *exothermic doublet*—that continues to supply fuel and oxidizer to the sheet via local mixing. Pressure contours pass through the sheet unaffected—attesting to the fact that combustion is an isobaric process. The exothermic doublet sheet is continually entrained into the mixing layer—thereby filling the products with vorticity, as predicted by Zel'dovich [17] in 1949.

The mass-fraction, $\mu(t)$, of fuel consumed by combustion of a 1-gram spherical TNT charge is shown in Fig. 5. Fuel consumption rates depend on confinement (chamber volume), with the unconfined case taking virtually an infinite amount of time to consume all the fuel.

Figure 6 displays the pressure histories generated by the detonation and combustion of a 0.8-kg TNT cylinder in a 16m³ chamber. The 3d-AMR simulation results are in good agreement with the experimental pressure measurement thereby validating the combustion model for this class of flows.

Conclusions

A theoretical model of combustion in spherical TNT explosions at large Reynolds, Peclet and Damk hler numbers is described. It is comprised of: (i) a *Multi-fluid Model* (consisting of the gasdynamic conservation laws for the mixture, supplemented by mass and energy conservation laws for each fluid, each containing the appropriate source/sink terms); (ii) a *Thermodynamic Model*, and a (iii) a *Combustion Model* (that takes into account sub-grid mass diffusion of F & A to form reactants, material transformation from reactants to products, and thermal equilibration of gases due to sub-grid heat diffusion). A key feature of this model is that combustion is treated as material transformations in the Le Chatelier plane rather than heat release. In fact, heat is not released; instead, combustion simply re-arranges the masses and energies among the fluids in an exothermic cell under the constraint of mass and energy conservation for the mixture (i.e., the mixture mass and total energy equations are devoid of sources).

In the limit considered here, combustion is concentrated in thin exothermic sheets (boundaries between fuel and oxidizer). The products expand along the sheet creating an *exothermic doublet* that continues to feed the sheet with fuel and oxidizer due to local mixing.

The Model presented here illustrates the link between turbulence (vorticity) and exothermicity (dilatation) in the limit of fast chemistry thereby demonstrating the controlling role that fluid dynamics plays in such flows.

References

- [1] Anisimov, S.I., & Zel'dovich, Ya. B., "Rayleigh-Taylor instability of the boundary between detonation products and gas in a spherical explosion", *Pis'ma Zh. Eksp. Teor. Fiz.*, **3**, 1977, pp. 1081-1084.
- [2] Anisimov, S.I., Zel'dovich, Ya. B., Inogamov, N.A. & Ivanov, M.F., "Taylor instability of contact boundary between expanding detonation products and a surrounding gas", *Shock Waves, Explosions & Detonations* *Prog. Astronautics & Astronautics Series*, **87**, AIAA, Wash., DC, 1983, pp 218-227.
- [3] Richtmyer, R. D., "Taylor Instability in Shock Acceleration of Compressible Fluids", *Comm. Pure Appl. Math.*, **13**, 1960, pp. 297-319.

- [4] Meshkov, E. E., "Instability of the Interface of Two Gases Accelerated by a Shock Wave", *Izv AN SSRE Mekhanika Zhidkosti i Gaza*, **4** (15), 1960, pp. 151-157.
- [5] Kuhl, A. L., "Spherical Mixing Layers in Explosions", *Dynamics of Exothermicity*, edited by J. R. Bowen, Gordon and Breach Publishers, Longhorn, PA (1996), pp. 291-320.
- [6] Ornellas, D. L., Calorimetric Determination of the Heat and Products of Detonation for Explosives: October 1961 to April 1982, LLNL, **UCRL-52821**, Livermore, CA, 1982.
- [7] Kuhl, A. L., & Oppenheim, A.K., Turbulent Combustion in the Self-Similar Exothermic-Flow Limit, *Advanced Computation and Analysis of Combustion*, ENAS Publishers, Moscow, 1997, pp. 388-396.
- [8] Kuhl, A. L., Ferguson, R. E., & Oppenheim, A. K. Gasdynamics of Combustion of TNT Products in Air, *Archivum Combustionis*, **19**(1-4), pp. 67-89, 1999.
- [9] Kuhl, A.L., Oppenheim, A.K., Ferguson, R.E., Thermodynamics of Combustion in a Confined Explosion, *12th All-Union Symposium on Combustion & Explosion*, **1**, Inst. Problems of Chemical Physics, 2000, pp. 182-184.
- [10] Gilmore, F., *Equilibrium Composition & Thermodynamic Properties of Air to 24000 K*, **RM-1543**, Rand, 1955.
- [11] Fried, L. E., *CHEETAH 1.22 User's Manual*, **UCRL-MA-117541** (rev. 2), LLNL, 187 pp., 1995.
- [12] Reynolds, W.C., *STANJAN Interactive Programs for Chemical Equilibrium Analysis*, Stanford, 48 p, 1986.
- [13] Colella, P. and Glaz, H. M., Efficient Solution Algorithms for the Riemann Problem for Real Gases, *J. Comp. Physics*, **59** (2), 1985, pp. 264-289.
- [14] Berger, M. J. and Colella, P., Local Adaptive Mesh Refinement for Shock Hydrodynamics, *J. Comp. Physics*, **82** (1), 1989, pp. 64-84.
- [15] Bell, J. B., Berger, M., Saltzman, J., Welcome, M., "Three-Dimensional Adaptive Mesh Refinement for Hyperbolic Conservation Laws," *SIAM J. Scientific and Statistical Computing*, **15** (1), 1994, pp. 127-138.
- [16] Brode, H. L., Numerical Solution of Spherical Blast Waves, *J. App. Phys.*, **26**, 766 (1955).
- [17] Zel'dovich, Ya. B., "K Teorii Goreniiya Ne Peremeshannykh Gazov" ("On the Theory of Combustion of Initially Unmixed Gases") *Zh. Tekh. Fiz.*, **19** (10), 1949, pp. 1199-1210.

Auspices

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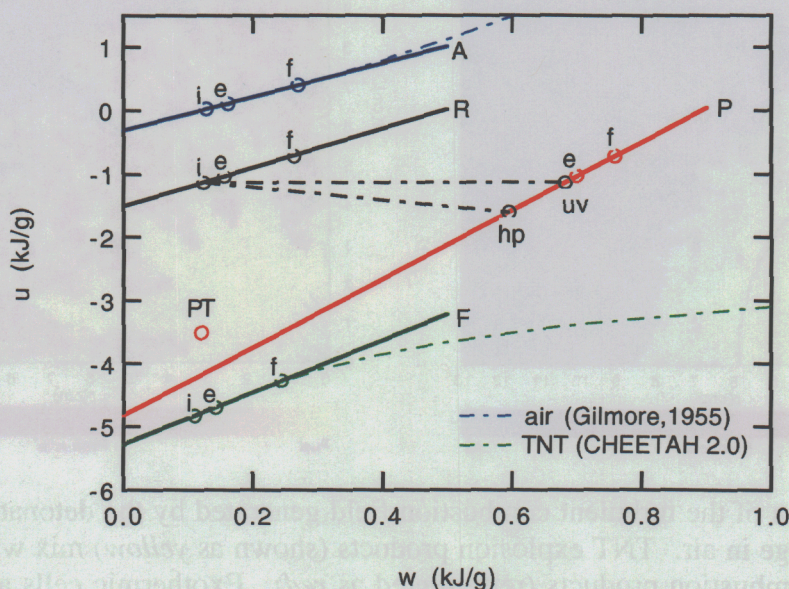


Figure 1. Le Chatelier diagram of states for combustion of Fuel-F (expanded TNT detonation products) with Air-A, forming stoichiometric Reactants-R, which transform into equilibrium combustion products-P.

Development of the Turbulent Combustion Layer

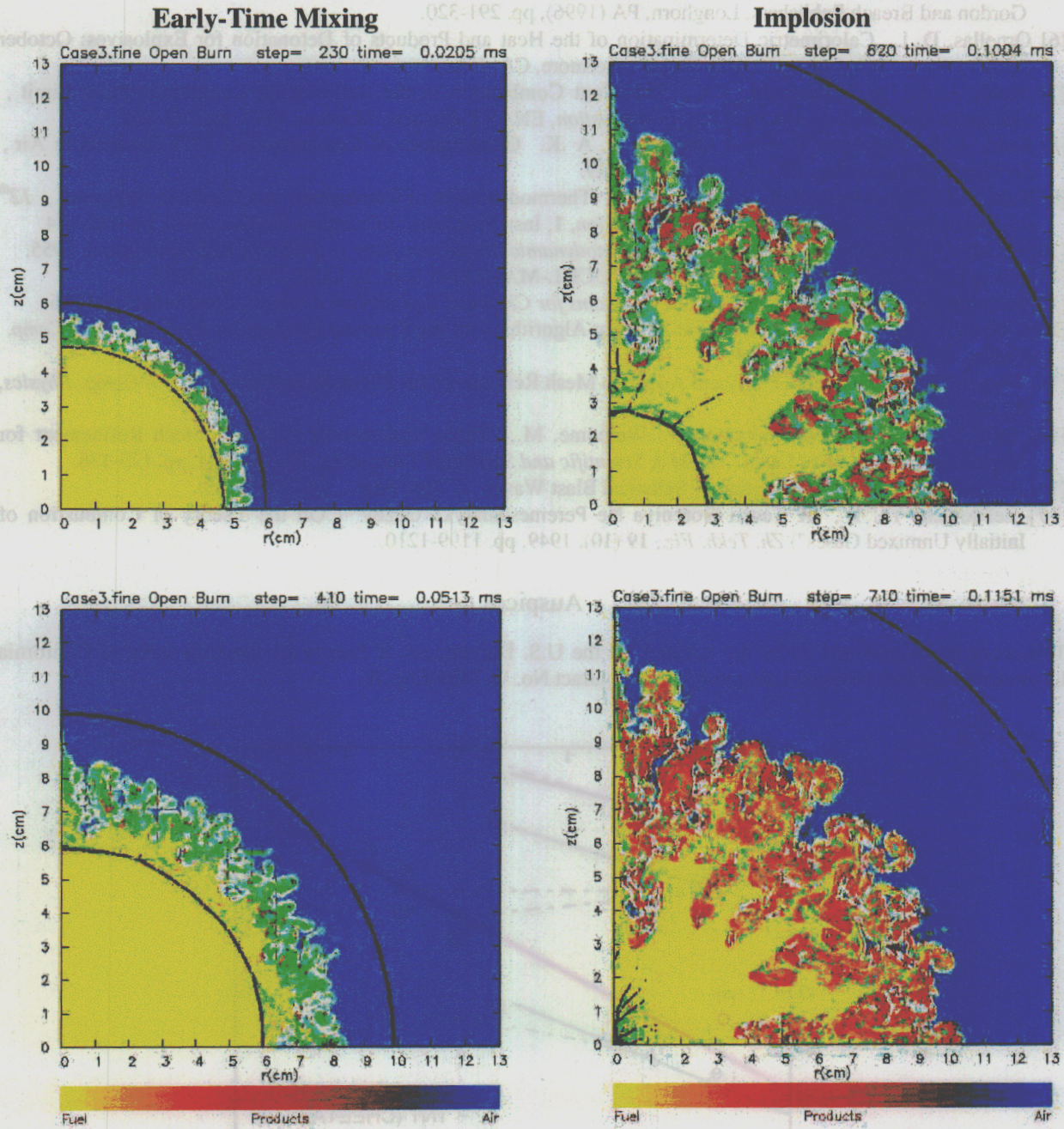


Figure 2. Evolution of the turbulent combustion field generated by the detonation of a 1-gram spherical TNT charge in air. TNT explosion products (shown as yellow) mix with air (depicted in blue) to form combustion products (represented as red). Exothermic cells are marked with white dots. Vorticity contours are turquoise (positive) and chartreuse (negative), while compressional dilatation contours are black.

Development of the Distributed Combustion Regime

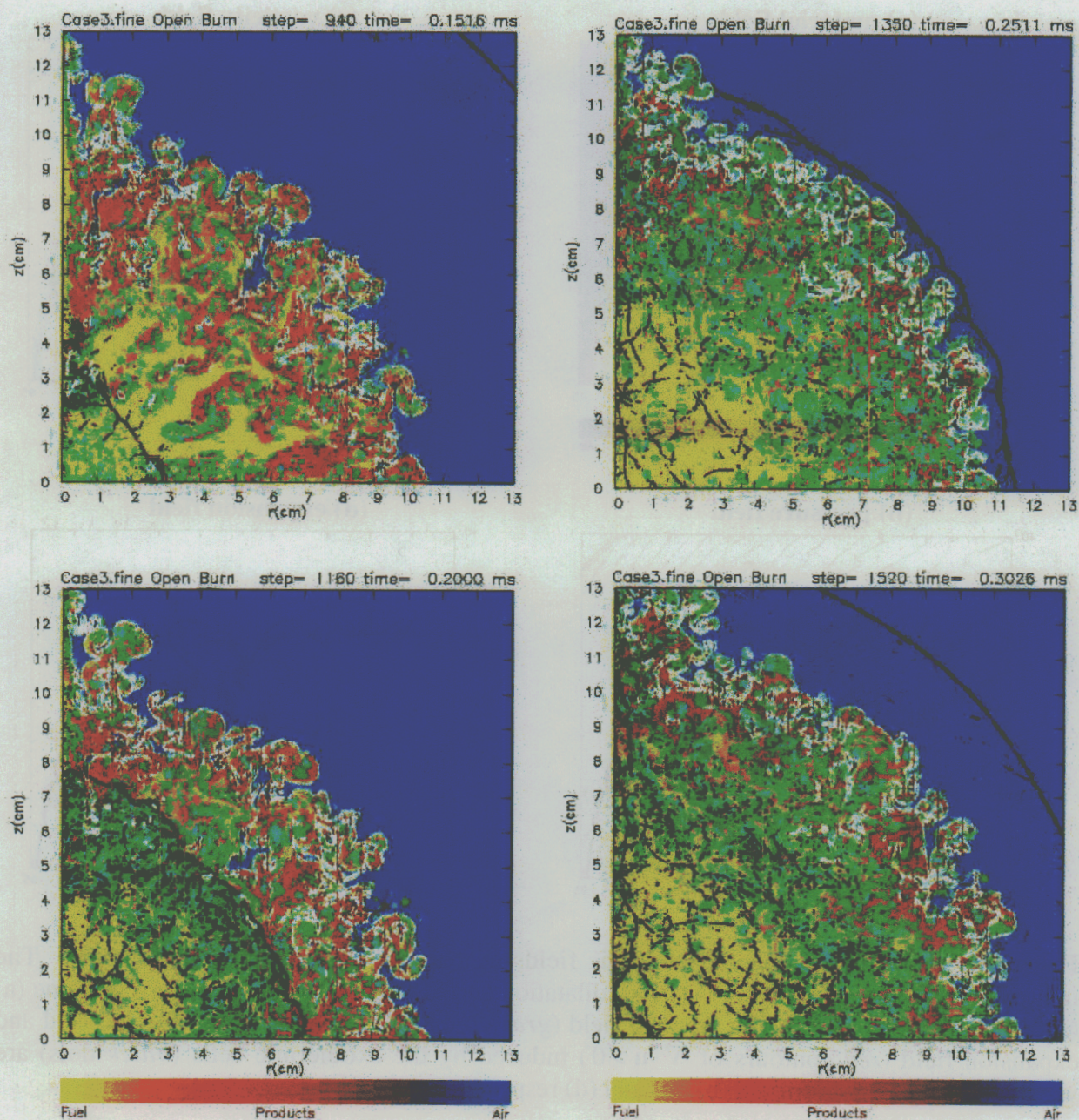


Figure 3. Emergence of the secondary shock from the mixing layer, leading to the emergence of a distributed combustion regime of energy deposition.

Exothermic Fields

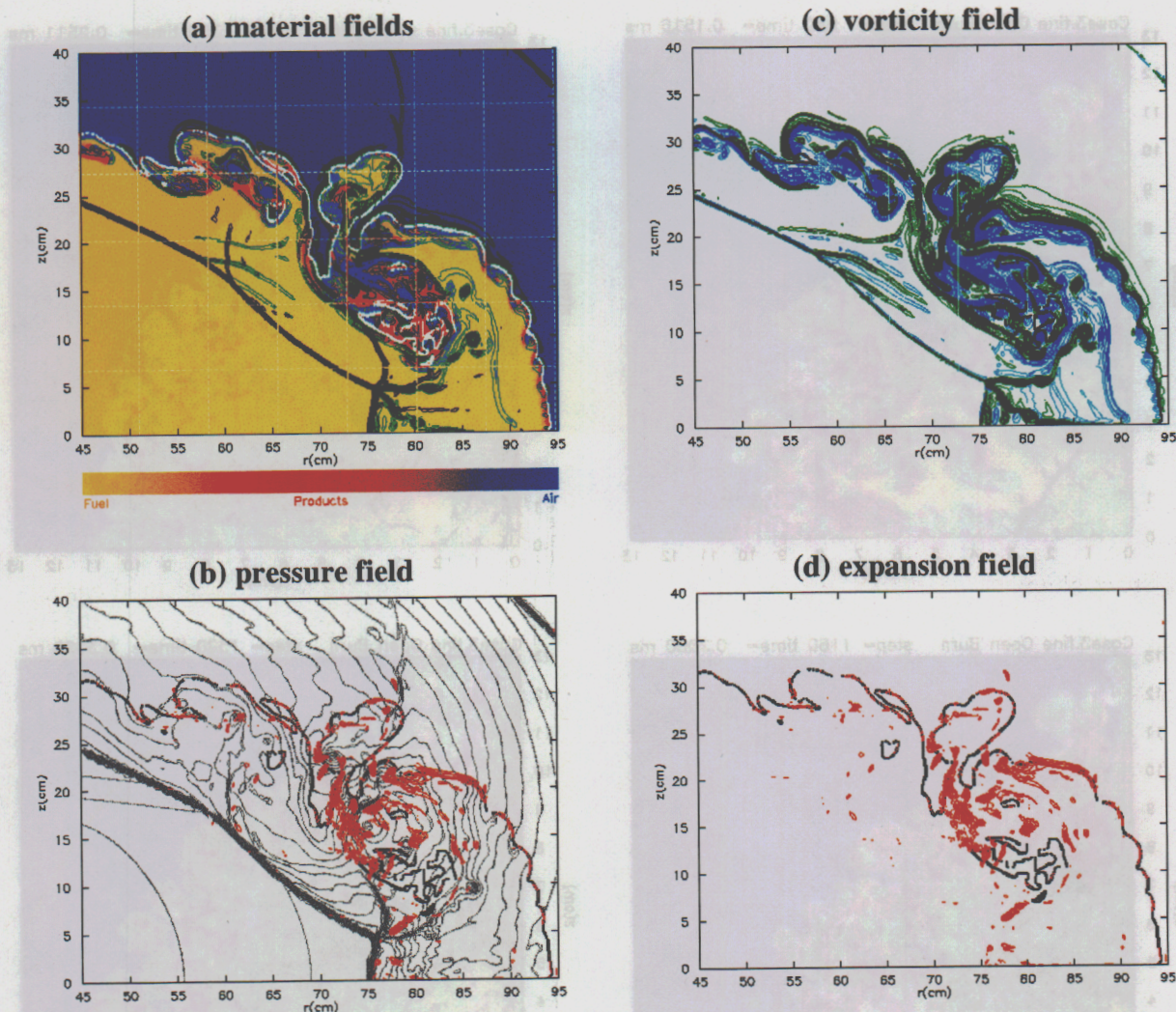


Figure 4. Visualization of the exothermic fields near a turbulent combustion structure. The material fields, with overlays of vorticity, dilatation and exothermic cells, are shown in frame (a) (same notation as Fig. 2). The pressure field (*gray* contours), along with the vorticity field and expansion field (*red* contours of $\nabla \cdot \mathbf{u} > 0$) induced by the exothermic cells (*black* dots) are visualized separately in frames (b), (c) and (d) respectively.

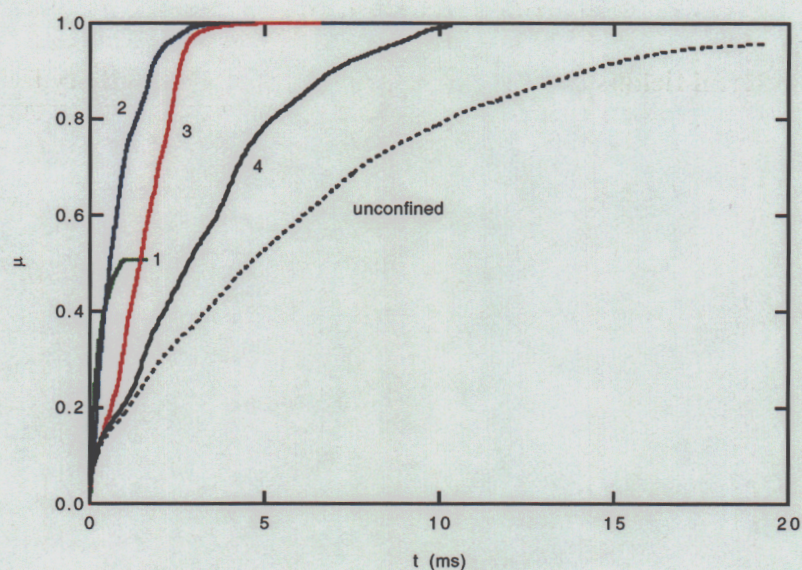


Figure 5. Mass-fraction of fuel consumed during combustion of a 1-gram TNT charge in different chamber volumes (1=0.7l, 2=6l; 3=50l; 4=400l) compared with the unconfined case.

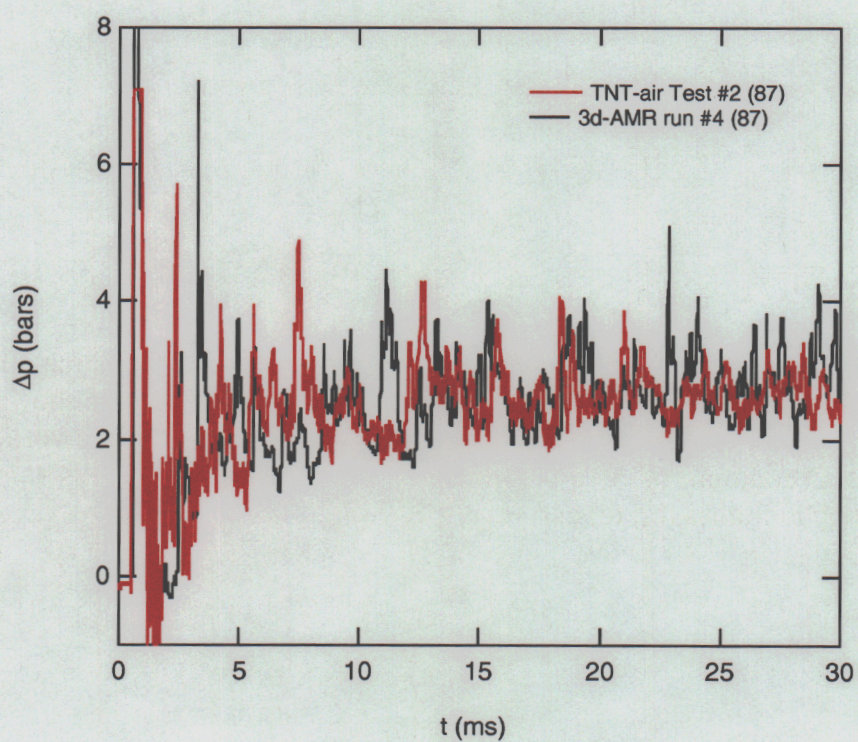


Figure 6. Comparison of a static pressure history from a 3d-AMR calculation with a pressure measurement for combustion of a 1-kg cylinder of TNT in a 16m³ chamber.

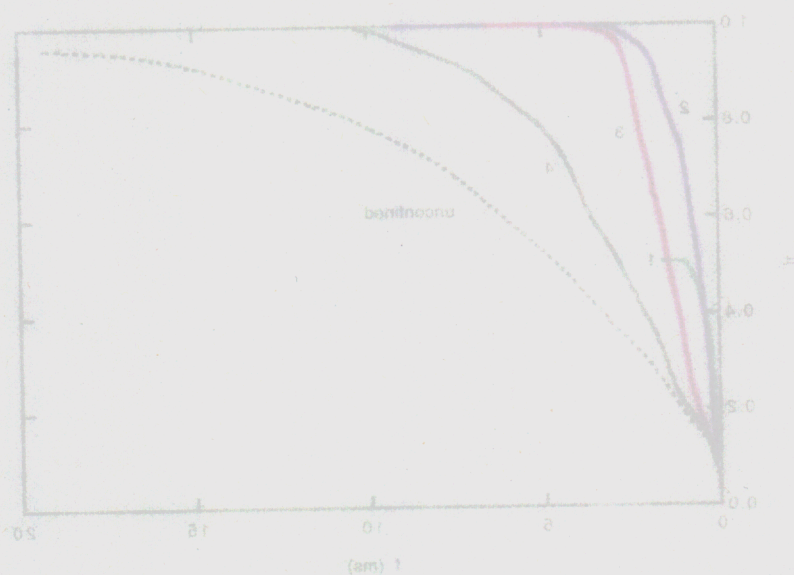


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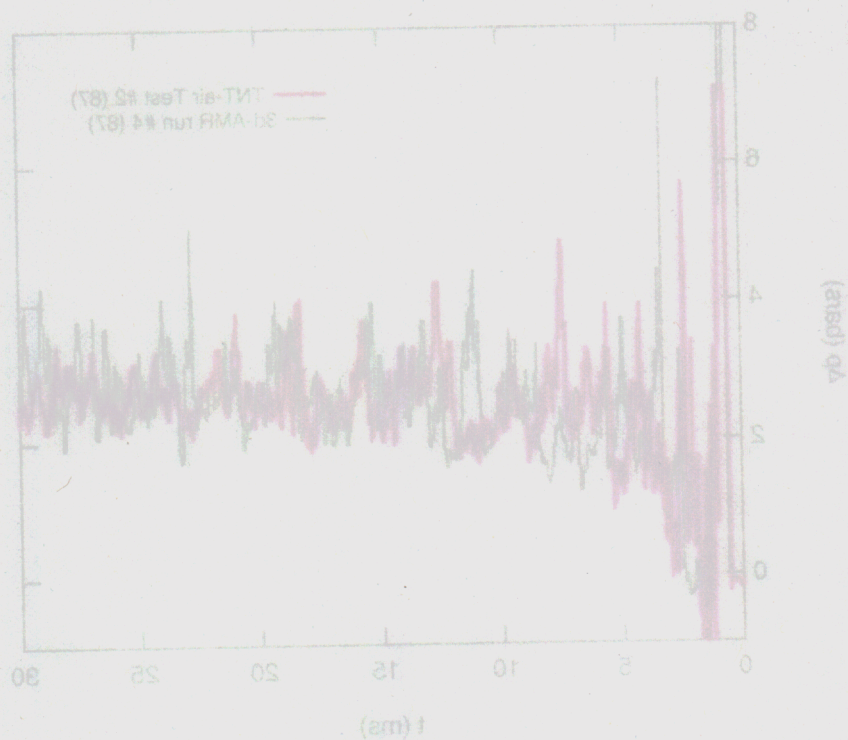


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